### **BOUT:**

## **Boundary Turbulence Simulations Code** in Magnetic Fusion Devices

X.Q.Xu

Lawrence Livermore National Laboratory
University of California
Livermore, CA 94550, USA



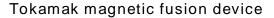
Presented at
BlueGene/L workshop
August 13-14, 2002
Lake Tahoe, CA, USA

## **BOUT Developer Team and Their Quest**

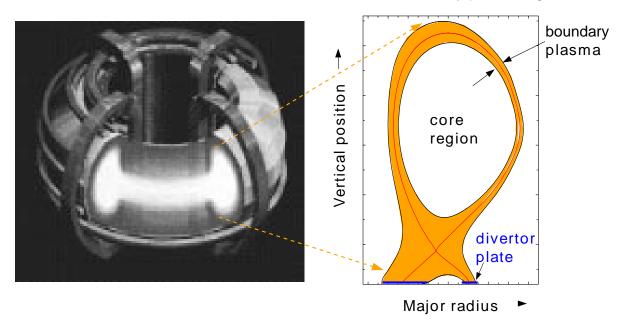


Ron Cohen
Bill Meyer
LLNL
Bill Nevins
LLNL
Tom Rognlien
LLNL
Marv Rensink
LLNL
Xueqiao Xu
LLNL
D. Ulrich
CSUS

Phil. Snyder GA
Sergei Galkin UCSD
S. Krashenninikov UCSD
Jim Myra Lodestar Inc.
Ralf Kleiber IPP/Germany
P. Catto/A. Simokov MIT

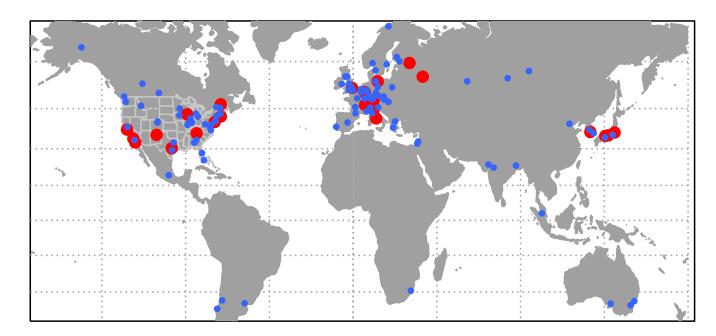


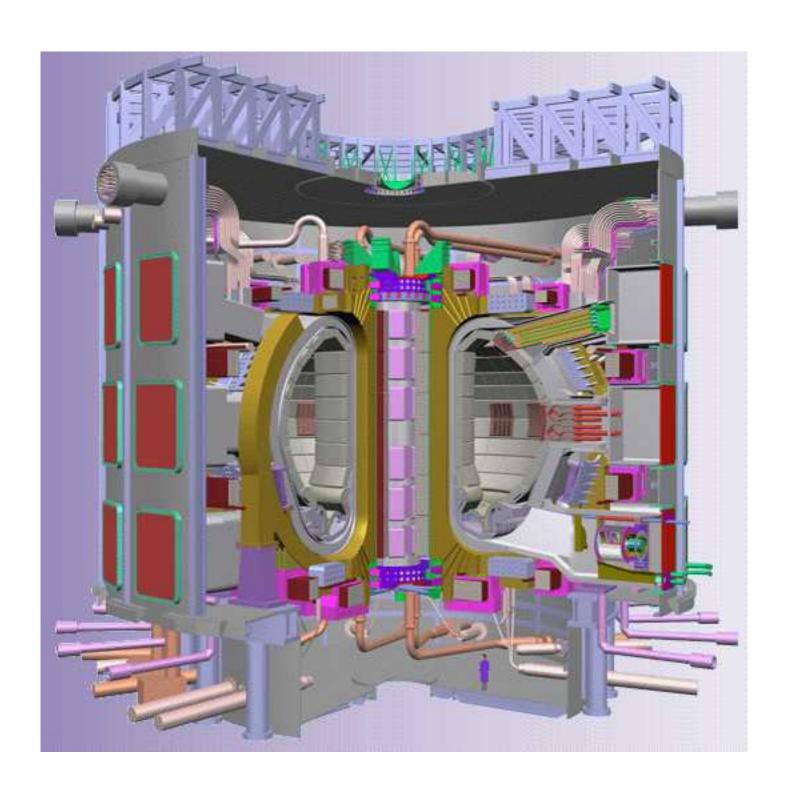
#### Simulated boundary-plasma region



#### **SCOPE OF THE WORLD FUSION PROGRAM**

- At last count 33 countries, 180 institutions (67 in the US)
- Emphasis Varies
  - US priority to science mission for now, US has withdrawn from burning plasma project - ITER
- EU, Japan give priority to energy mission





#### **FACILITIES AND INFRASTRUCTURE ARE EXTENSIVE**



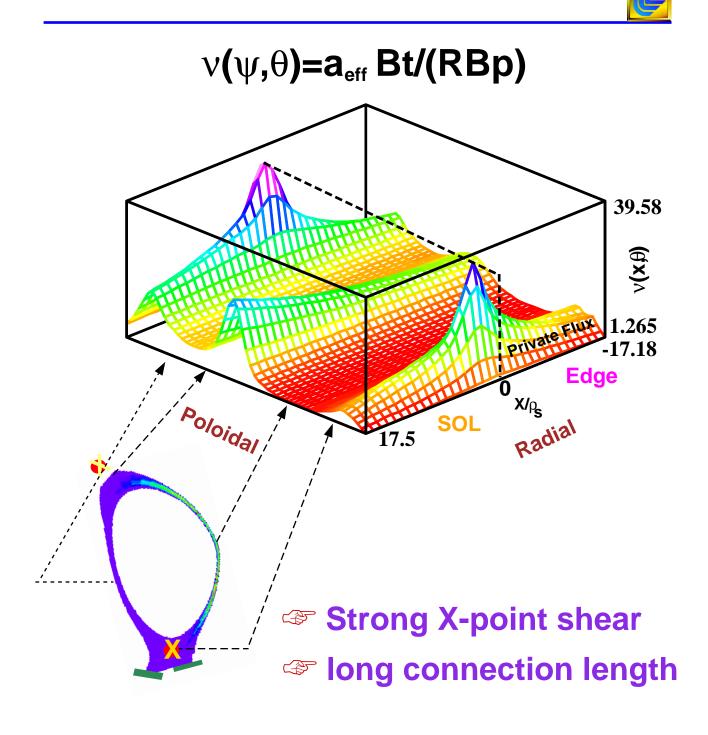
# **BOUT** is 3D EM Boundary Plasma Turbulence Code



- Boundary Plasma Turbulence has a different characters than in the core and play an important role in core confinement
- BOUT is an unique code to simulate boundary plasma turbulence in a complex geometry
  - → Observed large velocity shear layer
  - → Proximity of open+closed flux surface
  - → Presence of X-point
- BOUT is being applied to DIII-D, C-mod, NSTX, ITER for Snowmass, ...

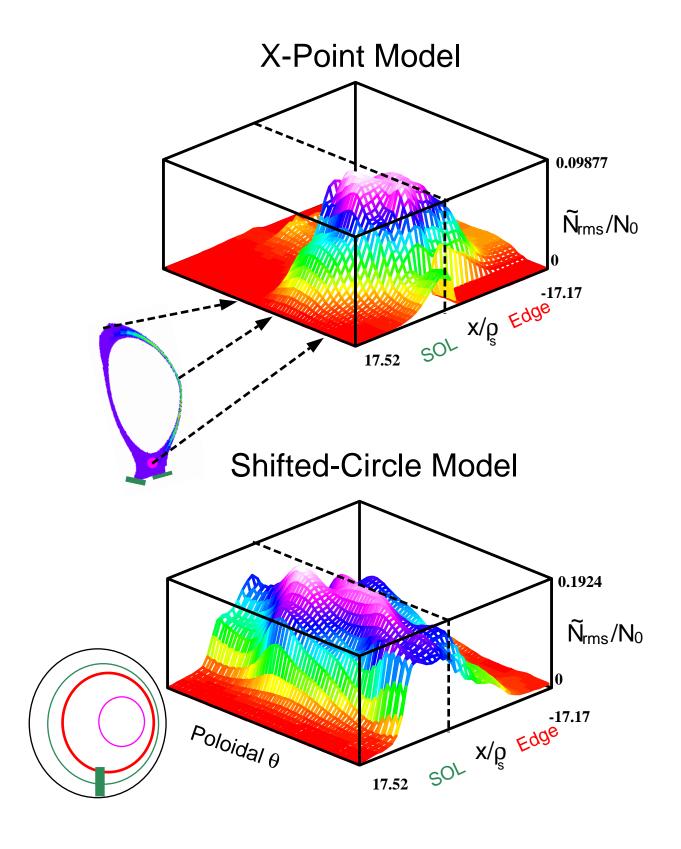


# Local Safety Factor, ν(ψ,θ), has strong variations near X-points that affect mode



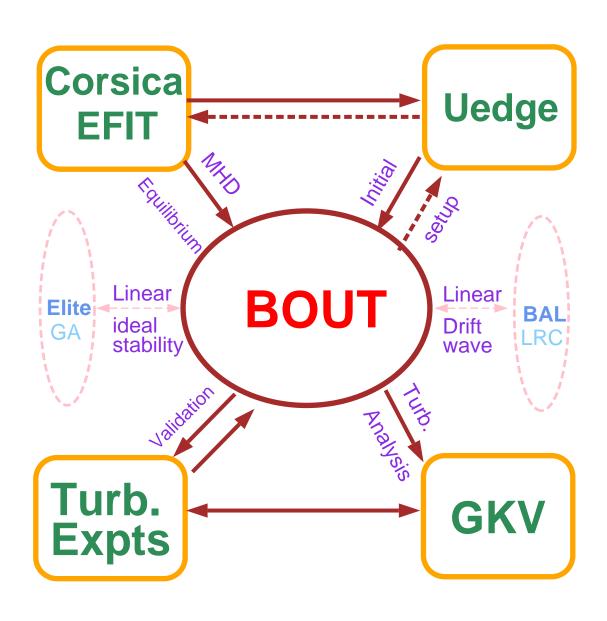
## Density fluctuation is ballooning for X-point geom. vs. flute for shifted-circle





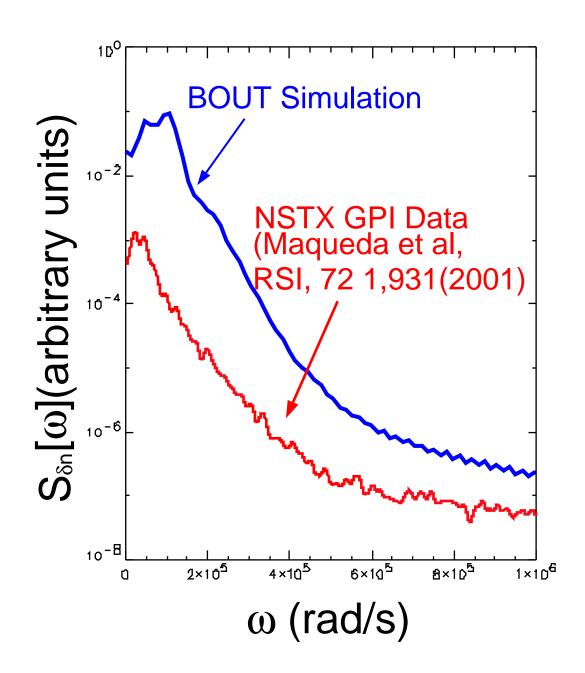
# A suite of the codes work together to make BOUT simulation results similar to real experiments





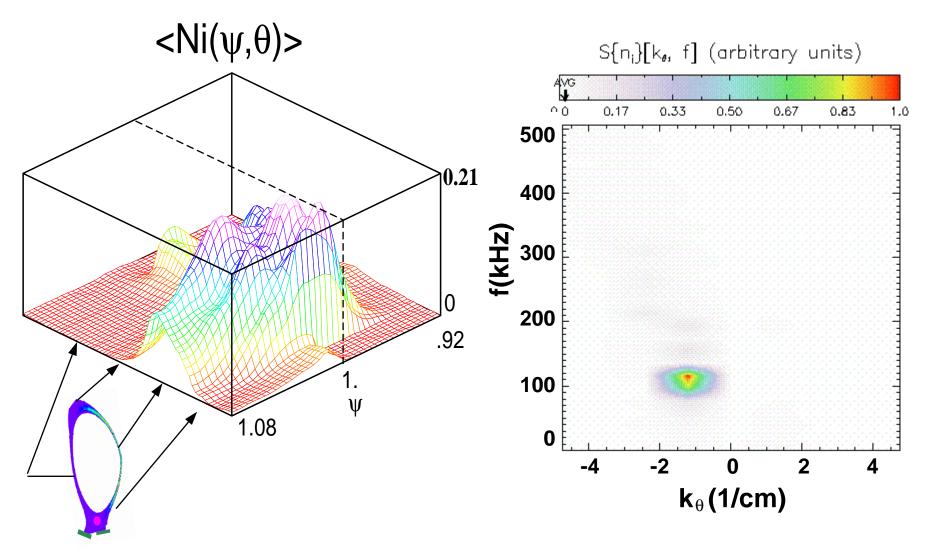
## **BOUT** shows similar frequency spectrum as Gas Puff Image





### **BOUT Simulates Mode Similar to C-Mod Quasi-Coherent Mode**

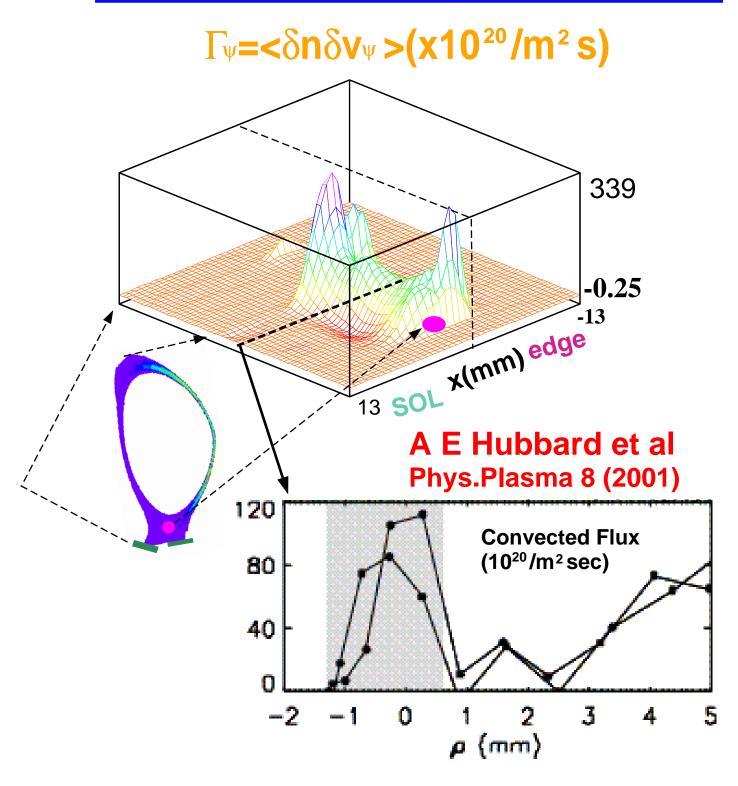




Code Result well Localized in f and k<sub>θ</sub> resembles PCI measurements

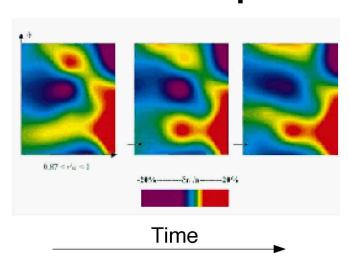
# Particle Flux $\Gamma_{\!\!\!\!/}$ is consistent with probe measurement near midplane region

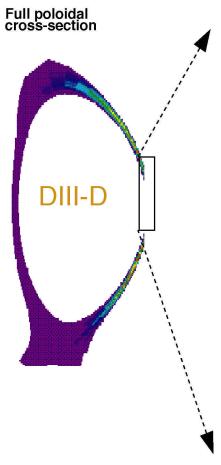




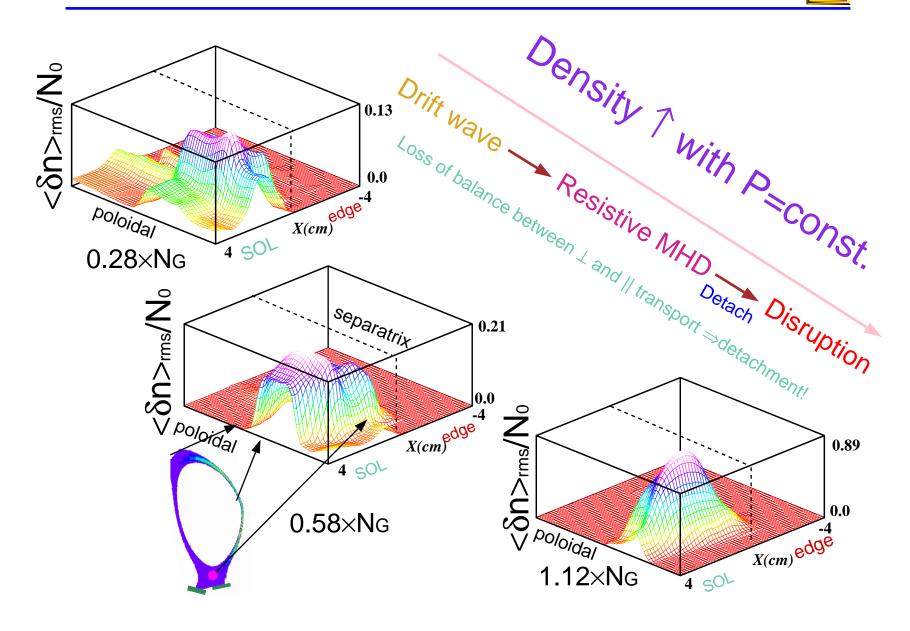
L-Mode Edge Turbulence in DIII-D Full poloidal

**BES Expt.** 



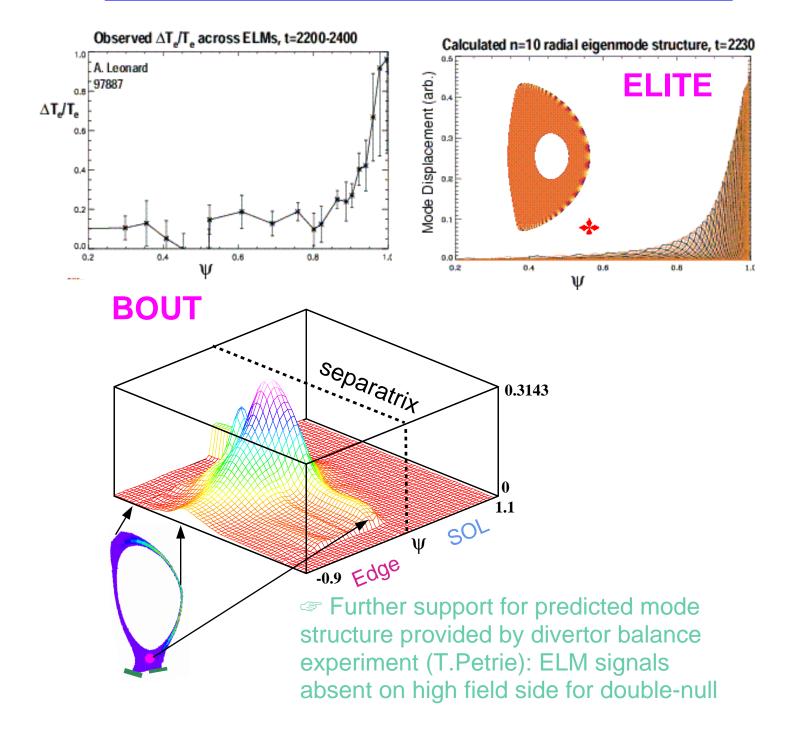


## **Dansity Limit:** High collisionality ⇒ fluctuation level/transport ↑ and parallel correlation length ↓



## Calculated Mode Structure from **BOUT and ELITE Consistent** with Observed DIII-D ELM Depth

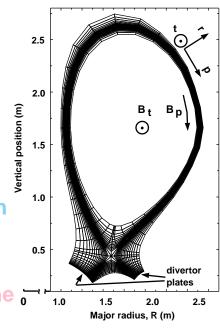


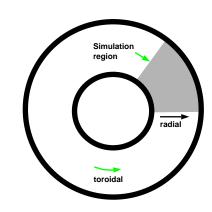


### BOUT is a parallelized 3D nonlocal electromagnetic turbulence code using MPI



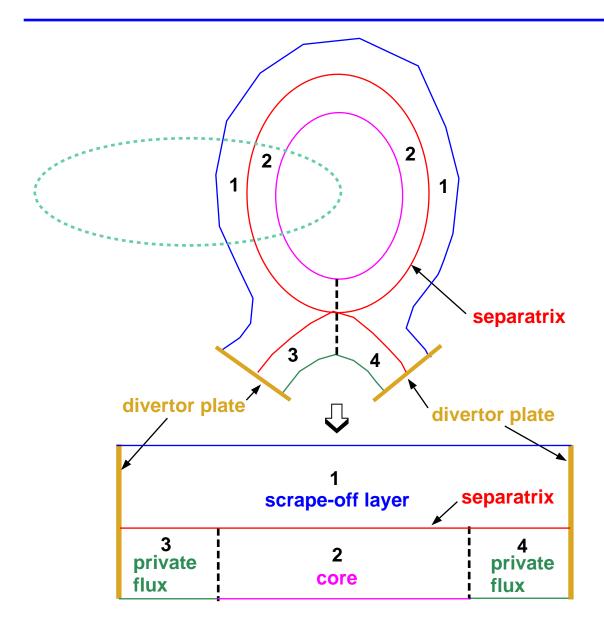
- **The BOUT code solves for the plasma fluid equations in a 3-D toroidal segment.**
- **BOUT** uses a fully implicit Newton-Krylov solver PVODE.
- **BOUT** is a parallelized code based on domain decomposition that uses the MPI system.
- BOUT has been tested on Linux PC clusters, Sun and DEC workstation clusters, and on the NERSC IBM SP and Cray-T3E.
- Parallel for one direction; parallelization in second direction is under way, will use~1000---10000 PEs
- Mflop/s rates achieved is typically ~ 5---10% on IBM SP



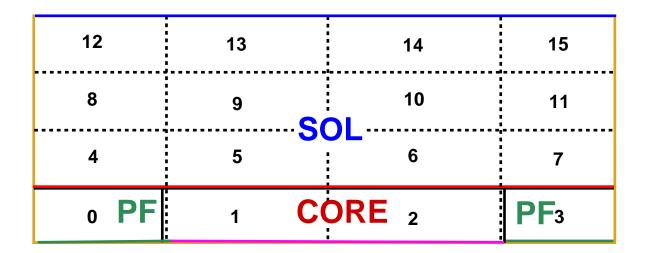


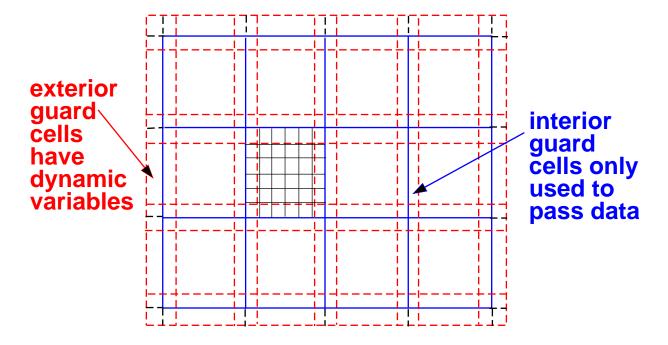
# The poloidal plane is divided into four main regions for the domain decomposition model



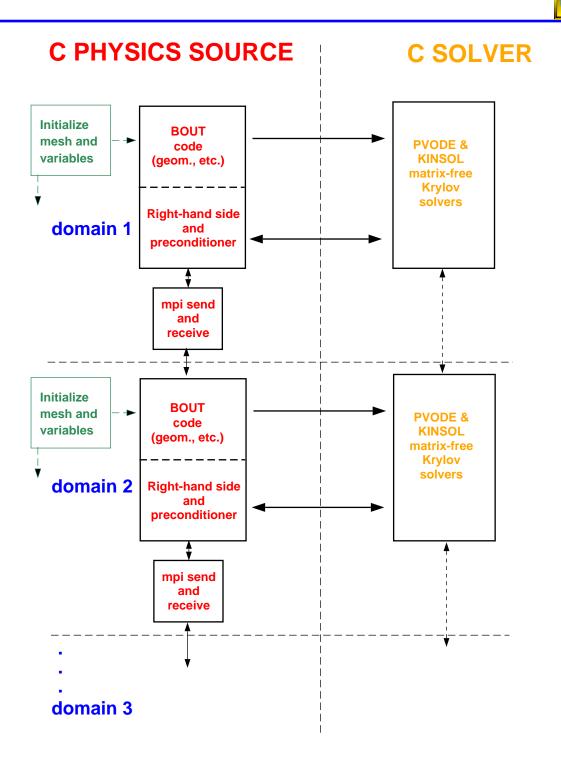


# Each of four main regions can be futher subdivided for the domain decomposition model

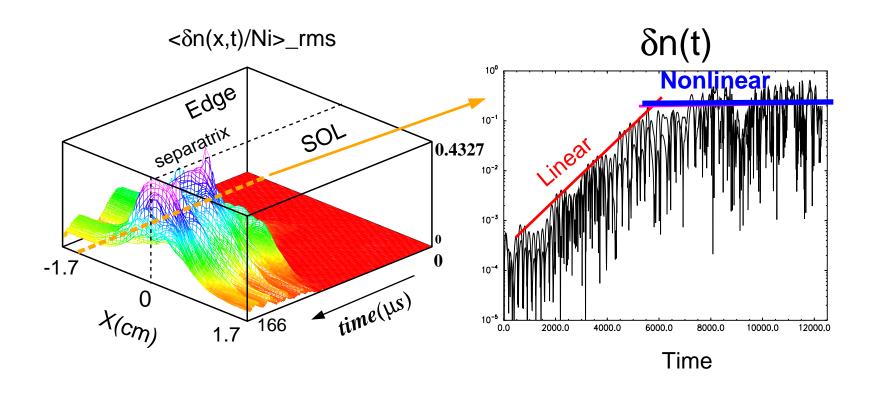




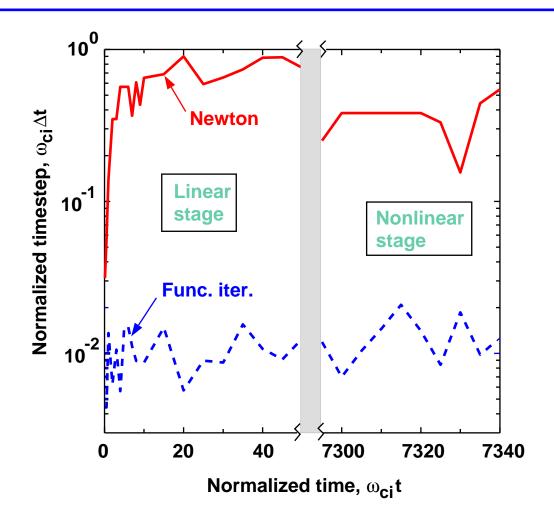
# Schemic showing the two major components of parallel BOUT Code as replicated on each domain processor



# Time history of linear growth and turbulence saturation



# Time step showed in BOUT over the course of a time-dependent simulation showing improvement with Krylov vs. func. iter.

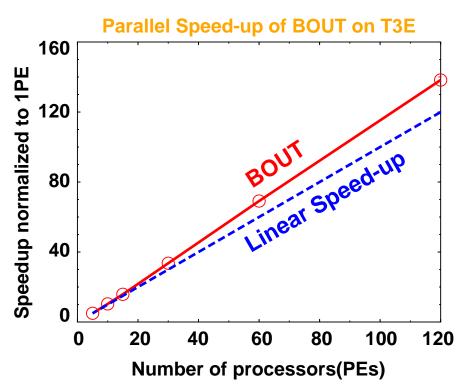


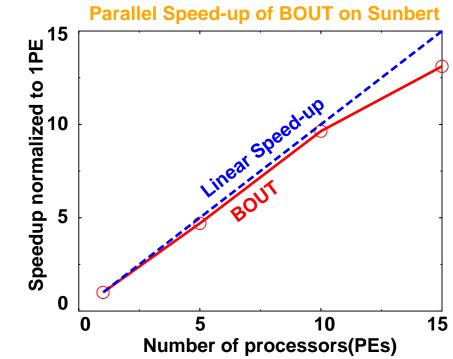
## Comparison of Adams Predictor-Corrector and Newton-Krylov (BDF) Statistics in Linear Stage of the Simulation

	Number of	Number of		Observed
Method	RHS evaluations	time steps	Average ΩciΔt	∆torder
One-step P/C	6212	5756	0.01	1
BDF Newton	1091	115	0.7	3-4

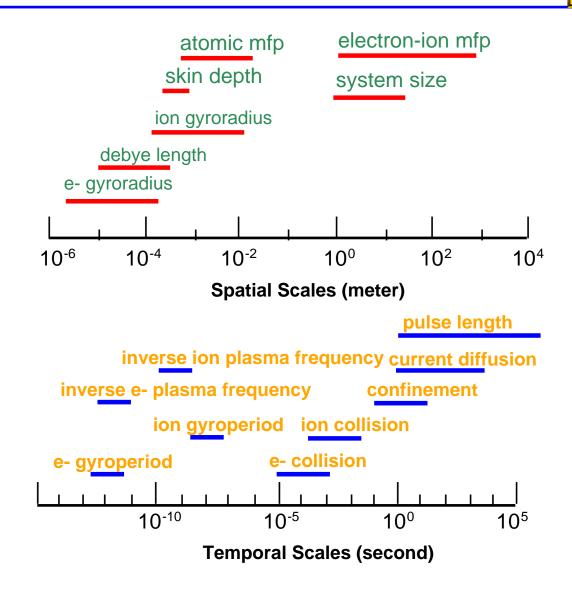
## **BOUT results show an almost linear speedup on T3E and Sunbert**







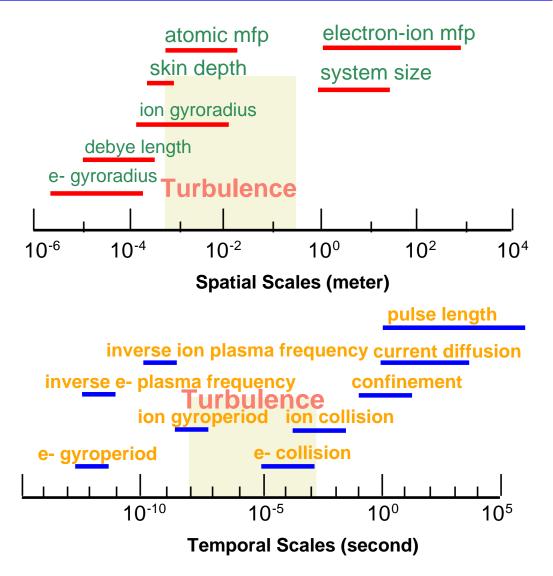
## Huge range of spatial and temporal scales is a challenge to theory and simulations



Overlap in scales often means that strong theoretical ordering is not possible

## BOUT simulates only part of boundary problems---Turbulence





It is even not possible to simulate whole boundary physics yet on today machines

## BlueGene/L will provide enough computing power to simulate boundary physics

#### A proposed Kinetic BOUT code: 2V3D

- Resolution  $30\times30\times100\times100\times1000\sim10^{10}$ ,  $\Delta x \sim 1$ mm, ion gyroradius spatial scale,  $\Delta t \sim 10^{-8}$  second, Alfven time scale
- Time ~ 10 --- 100 ms, Thus number of timestep ~  $1\times10^6$  ---  $1\times10^7$
- **⊘ Number of operation/grid point/step ~ 1000**
- Total operations count to carry out the simulations ~10<sup>19</sup>---10<sup>20</sup>
- With a 100 TF machine, the time required  $\sim 10^{19}$  ---  $10^{20}$  /( $10^{14} \times 3600$ ) $\sim 30$  --- 300 hours

### Issues of BOUT performance on BlueGene/L



#### **38** The division of work for BOUT on IBM SP ~ 100 PEs:

- > 80% for evaluating the BOUT physics equations,
- > 1% for I/O,
  - ⇒ a pointer variable is set so that each processor only reads a subset of the data needed for its domain.
  - each processor writes and reads its own dump file for the data in its domain for restarting the problem.
- > 12% for internal PVODE calculations,
- > 6% for interprocessor MPI communications,
- > 1% for other overhead costs,
- > 1% variation for the load balance among processors.

#### **38** We anticipate use ~10000 PEs on BlueGene/L,

- > ~ a flux tube per PE
- > Issues:

Parallel I/O:

Communications: Latence & bandwidth

File management:~1000-10000 files per simulation

Storage: ~ 1TB of data per simulation

**Unknown:**